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A Sampling of Multiscale Material Simulation at Sandia National Laboratories

"Microsystems and Beyond"

Sandia Science Day

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John B. Aidun, Manager
Computational Materials and Molecular Biology, 9235

CCIM
COMPUTATION, COMPUTERS, INFORMATION AND MATHEMATICS
National Leadership in High Performance Computing

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

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Notes from Previous Slide

A handful of research projects have sprung up at Sandia over the last year, or so, that are each focused on developing various aspects of multiscale material simulation capabilities.

I'll begin by quickly going thru several slides to give you the motivation for Sandia's strong interst in research on materials.

I'll move on to summarize why the multiscale material methods under development will be important to advancing our understanding of materials and, in turn, important to Sandia's core programmatic efforts.

(segu.) Among the DOE DP labs Sandia is known as the Engineering Lab.

I think you all know that the engineering we do is not routine – we can't look it up in the handbooks . . .

Sandia: The Extreme Engineering Lab

Extreme sports athlete Dave Mirra

To fulfill our National Security mission, we develop systems and components designed to perform extreme applications, under adverse conditions.

The duty cycle can include damage, crush and failure;

melting; decomposition – or just plain old age.

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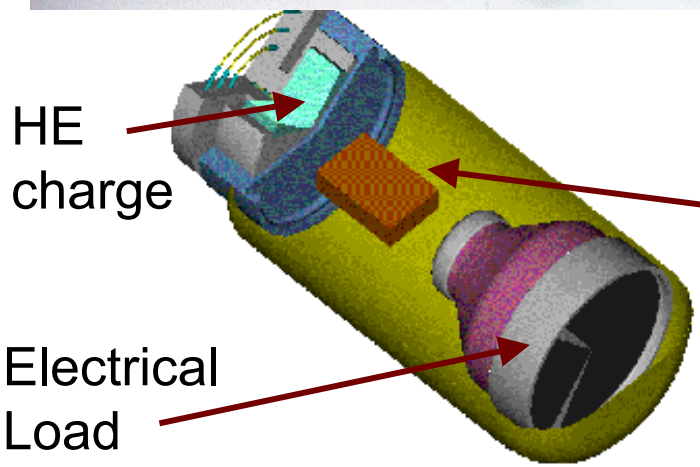
Notes from Previous Slide

. . . In fact what we do is best described as Extreme Engineering.

Example Applications I



Extremely Tough:

- Earth penetrator bombs
- Radiation-hard microelectronics
- Explosive Destruction System

Extremely Sensitive:

- Sensors
- Explosives Sniffer

Extremely Powerful:

- Ferroelectric ceramic power supply – explosively driven
- Pulsed Power Z-Machine

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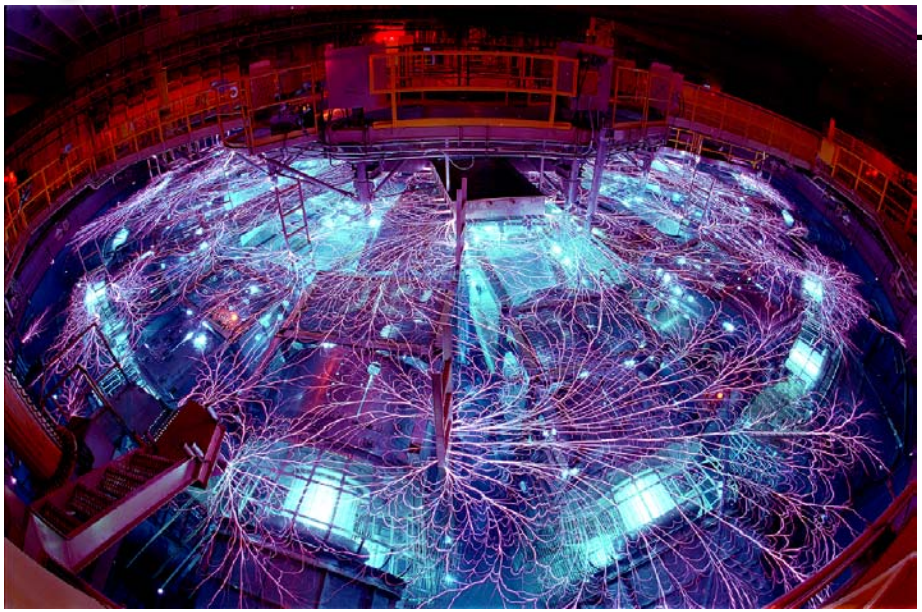
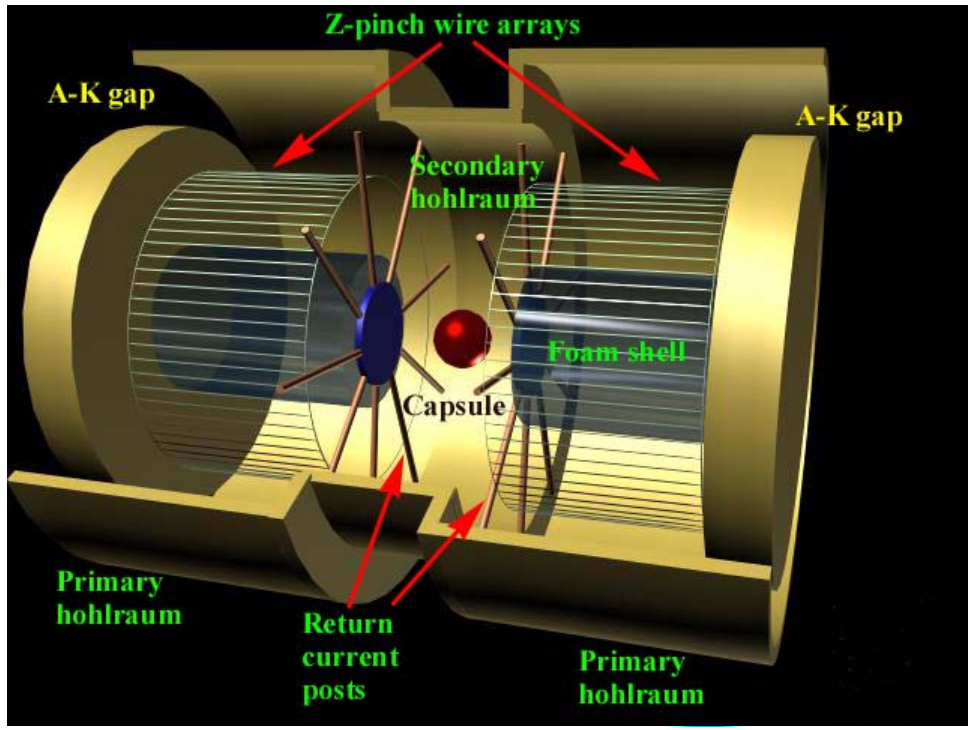
Pulsed Power & Inertial Confinement Fusion (ICF)



- ICF is a goal at Sandia National Labs
- Pulsed Power Technique using Z-machine

Wire arrays explode, creating a plasma sheath, which implodes and stagnates.

Resulting X-rays strike capsule, generating fusion reaction.



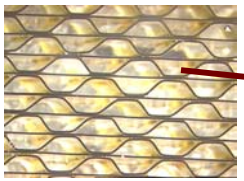
Notes from Previous Slide

ICF is still off in the future, but the Z machine is being used now for path breaking materials experiments.

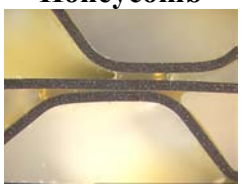
Materials modeling and simulation over and extreme range of conditions are indespensible for both designing and analyzing pulsed power experiments on Z

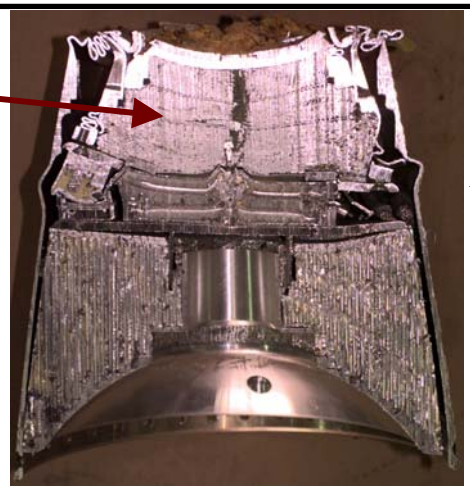
Need EOS, electrical and thermal conductivities, radiation opacities for metals and alloys from 2 x solid density down to 1% and from cryogenic Temp up to several eV [1eV = 11,600 K, or 2 x (surface of the Sun)]

Example Applications II



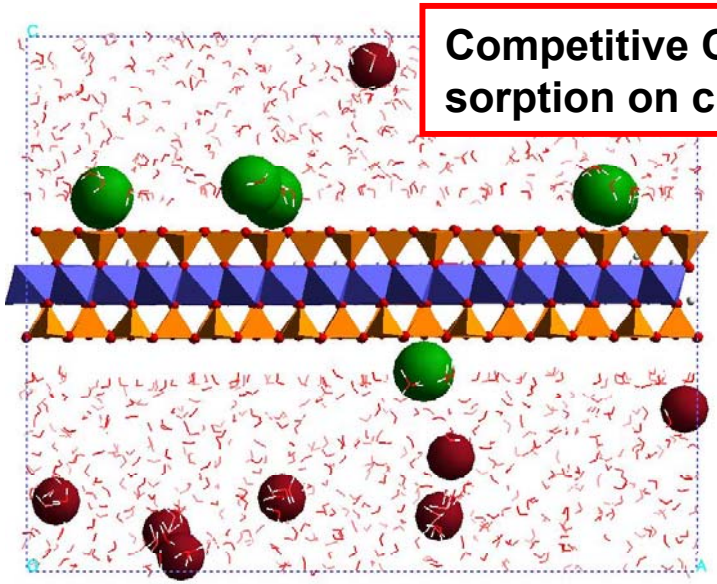
Aluminum Honeycomb





Extreme Insult Resistant:

- Aluminum Honeycomb energy absorber
- Engineered Stress Profile Glass
- Architectural Surety



Competitive Cs and Sr sorption on clay mineral

Extreme Effectiveness:

- Environmental remediation
- Decontamination Foam

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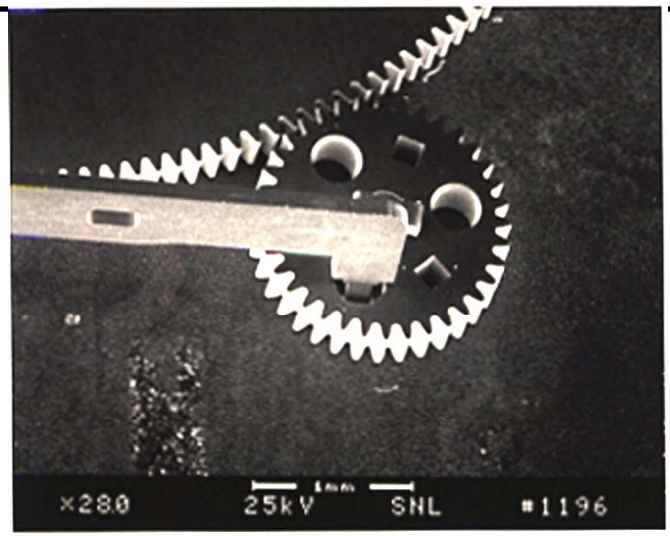
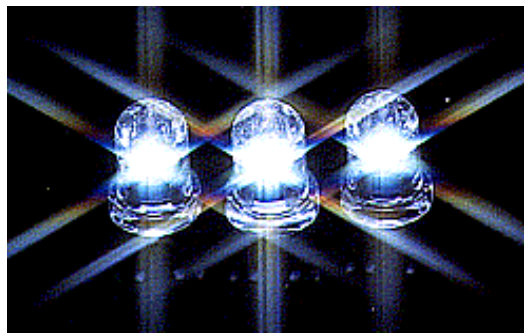
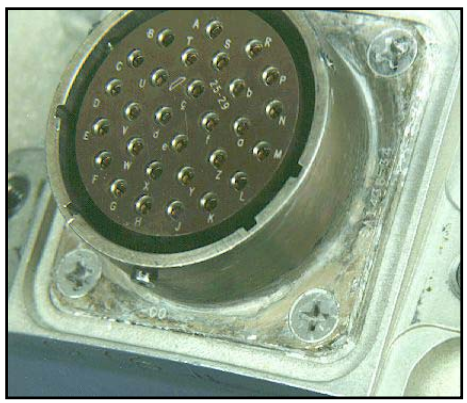
Example Applications III



Extremely Small & Efficient:

- Microsystems & Nanotechnology
- Solid State Lighting





Extremely Reliable:

- Electrical Connectors
- Bonds
  - Solder Joints
  - Adhesives Joints
  - Brazes and Welds

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Notes from Previous Slide

(bonds) We even have to engineer better bonds and joining processes.

Sandia: A Materials & Engineering Lab

- Extreme Engineering requires understanding and controlling the properties and behavior of materials.
  - In turn, this often requires understanding and controlling processing, which determines many aspects of material performance.
- Consequently, materials research is a big part of Sandia's Science & Technology efforts.
- **Computer modeling and simulation** is an integral part of the materials research we pursue.
  - It goes hand-in-hand with theory, experimentation, synthesis, and measurement.

Notes from Previous Slide

Extreme engineering relies on the strong science base at Sandia for its success.

M&S – complement to expt. and theory for nonlinear and collective phenomena.

– provides information on performance under conditions that are difficult or impossible to achieve and for materials that are too hard to handle due to size, stability (non-existent), or harzards.

(segu.) We continually expect more performance from materials for our applications.

Drivers for Ever-Increasing Goals for Materials Performance

- Continually evolving National Security needs .
- Technological Goals:
  - Smaller; Lighter
  - Higher Speed; Higher Efficiency; Higher Sensitivity
  - Greater Economy
  - More versatile; More robust in severe environments
- To meet new performance goals, we increasingly look to computer modeling & simulation to quickly provide accurate information on properties and behavior of materials, *both existing and imagined*.

Why Multiscale Material Simulation?

- The **GOAL** for materials modeling & simulation is to be able to make good predictions for **REAL** materials.
- Need to identify & understand the fundamental events occuring in each material (type) for each application.
- Primary physical traits and chemistry are determined at the atomistic level.
- Each scale of **heterogeneity** introduces additional phenomena
  - Lattice Defects; Subgrain domains; Grain boundaries; Multiple phases; Micro-cracks

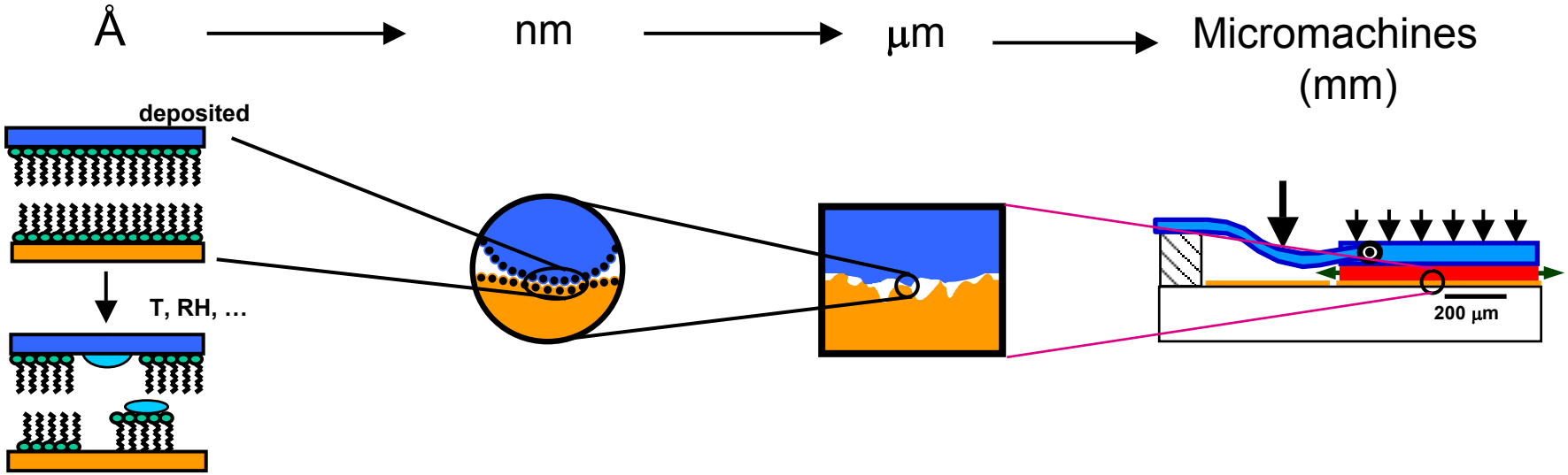
Notes from Previous Slide

The phenomena at each scale have their own characteristic length and time

(segu.) MEMS provide an example of multiscale phenomena.

Multiscale Material Phenomena – Interfacial Forces in MEMS

Linking length scales needed to understand and model adhesion, friction and wear:



- SAM coatings
- molecular structure
- stability and durability
- environmental degradation

- single asperity
- adhesion energy
- friction coefficient
- dynamics
- atomistic simulation

- multi-asperity
- surface morphology
- 'real' contact simulation

- design rules
- device models
- device performance
- reliability testing

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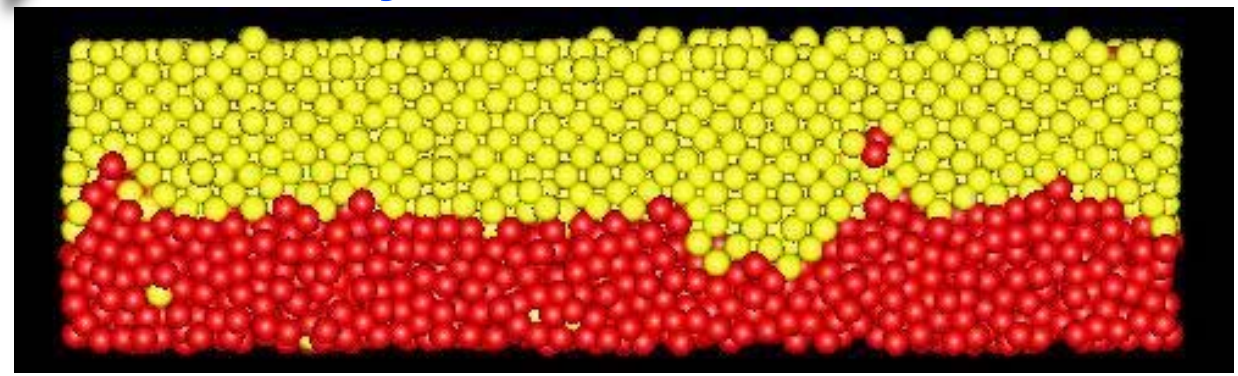
Notes from Previous Slide

[Go Right to Left]

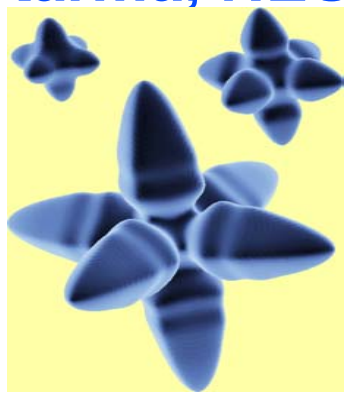
The thorough understanding needed to make a robust and reliable device requires treating the multiple scales of phenomena.

Sequential multiscale prediction of solidification rates in Ni

Jeff Hoyt, SNL; Mark Asta, NWU; Alain Karma, NEU

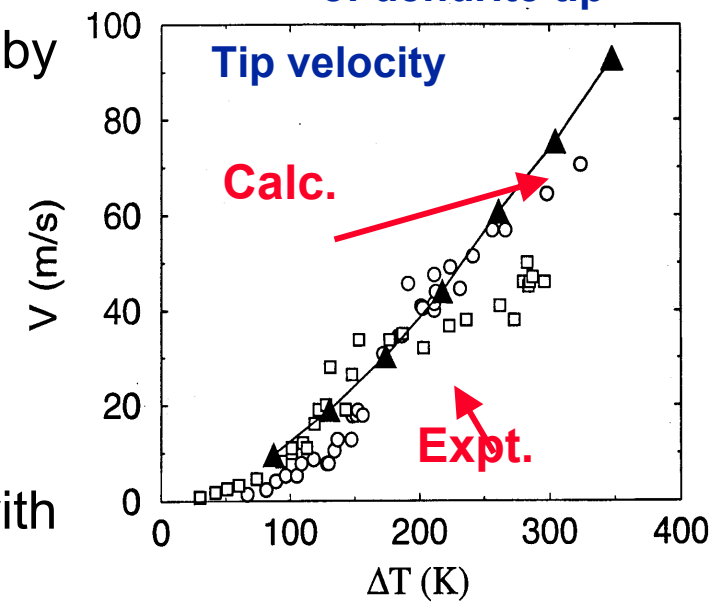


MD simulation of liquid-solid interface



Phase-field simulation of dendrite tip

- Molecular Dynamics simulations of solid-liquid interface predict parameters needed by phase-field model
  - Anisotropic interfacial free energy
    - *Novel fluctuation analysis*
  - Kinetic coefficients
- EAM potentials of Foiles, Baskes and Daw
- *Parameter-free* phase-field calculations predict dendrite tip velocity in agreement with experiment



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Notes from Previous Slide

I'll give two exampls of the power of multiscale modeling and simulation.

Sequential / traditional.

Atomistic simulation is used to compute values of material properties that are very hard or impossible to measure – solid-liquid interfacial free energy **and** its anisotropy.

These properties are required for the mesoscale phase-field model simulation

Plot is under cooling vs dendrite particle tip growth velocity

Scientific accomplishment: much better fundamental u'standing of metals solidification. Can now provide guidance for macroscale continuum engineering modeling of solidification.

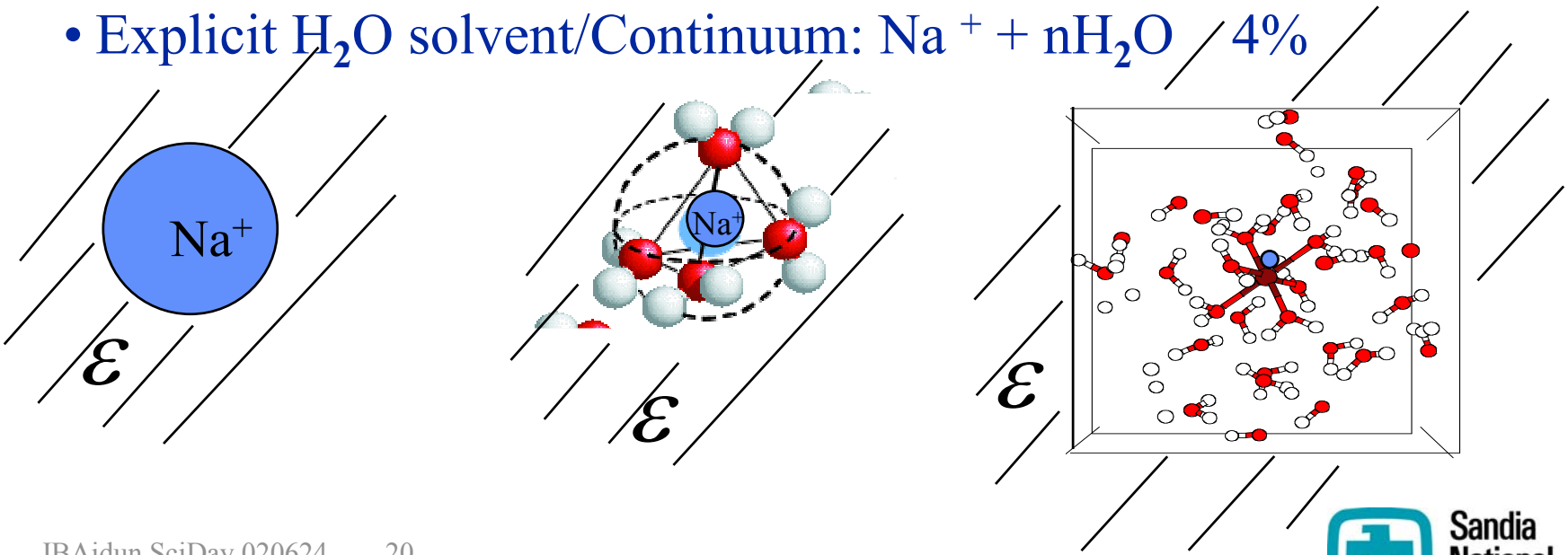
Technological application: processing (casting), welding, brazing.

[Ni blobs are magnetically levitated and undercooled, then touched with a needle to nucleate dendrites.]

Concurrent multiscale prediction of Hydration Energy for Sodium

S. Rempe (SNL), D. Asthagiri, L. Pratt (LANL), 2002

	$\Delta E^{hydration}$ Error
• Dielectric Continuum: $Na^+(aq)$	40%
• Explicit bound H_2O molecules: $Na^+ + nH_2O$	30%
• Explicit bound H_2O/Continuum: $Na^+ \; nH_2O$	15%
• Explicit H_2O solvent/Continuum: $Na^+ + nH_2O$	4%



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Notes from Previous Slide

The hydration energy is well-known. It is obtained from 19th century calorimetry measurement.

Four different approximations for the polarizability and structure of water

1. Continuum model of water as a uniform dielectric.
2. Shell of water molecules complexed to sodium ion
3. Shell of water molecules embedded in uniform dielectric continuum water
4. Extended system of water molecules embedded in uniform dielectric continuum water.

The Challenge: Size, Time, & Number

- Atoms to Objects:
  - nanometers, femtosec → cm, sec, Giga-Giga atoms
  - years: 10's of Msec
- Brute Force – State of the Art: F.F. Abraham (IBM)
  - 1 Billion atoms (Giga atom); a speck less than 1 μm^3
  - Highly simplified atomic interaction
  - Time interval 0.1 ns to 10 ns
- Moore's law will gradually extend the range of brute force.
- But brute force will never address the more subtle challenges associated with heterogeneity (next)

Notes from Previous Slide

Giga-Giga is a pinch of stuff. Giga is a billion. Giga-Giga is not Prof. Sagan's "billions & billions" but rather a billion TIMES a billion.

Abraham simulation is an impressive accomplishment.

Big simulations are v. interesting and informative, but they are only part of the answer.

Meeting the subtle challenges requires innovative science!

The Deeper Challenge to Multiscale Materials Simulation – The need for Science

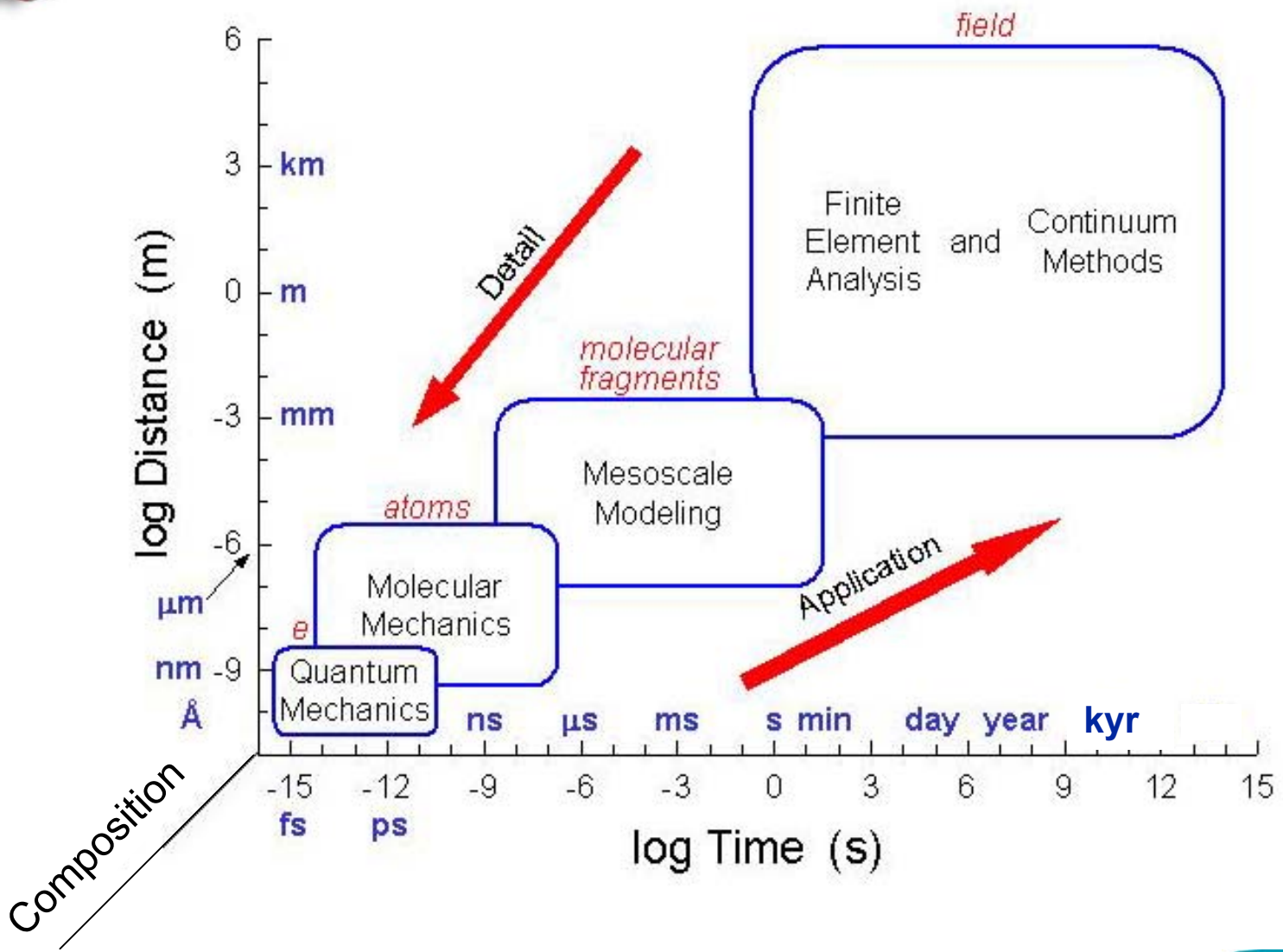
- Capturing diffusion, reactivity, and chemistry
  - This often requires Quantum Mechanics accuracy
- Attaining effectively very long times – Aging studies
- Applying high accuracy techniques when and where they are needed within a large system
  - "Interesting" events are infrequent.
  - Their time and location are not known.
- Removing or suppressing disturbances made by artificial boundaries in atomistic simulations.
  - Nanoscience is an easier target, in some ways.
  - Periodic Boundary Conditions – easy, but limited

Notes from Previous Slide

PBCs still have size effects

And they are not good for treating non-periodic systems like extended defects and **heterogeneous** materials

Computer Simulation L-t-x Array



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Notes from Previous Slide

The regimes of simulation methods:

Large to small:

1. Components, devices and systems.
2. Material Microstructure
3. Atoms
4. Electrons

Composition axis brings chemistry into the picture.

Classes of Simulation Methods

Quantum (nm, ps)

- Q.Monte Carlo
- Q.Density Functional Theory
- Tight Binding

Molec. Modeling (mm,ms)

- Molecular Dynamics
- Atomistic Monte Carlo (MC)
- Molecular Statistical Theory

Green: PDE methods

Mesoscopic (mm, s)

- Dislocation Dynamics
- Lattice Gas
- Cellular Automata
- Kinetic MC/Potts
- Coarse Grained MD
- Phase Field Models

Continuum down to (μm, μs)

- Finite Element Method
- Finite Difference
- Boundary Element
- Finite Volume
- Particle-in-Cell
- Transform methods

Notes from Previous Slide

TB – parameterized Quantum. A fast interpolation method.

There are a variety of good methods, but applying any of them to a new class of problems requires innovation and art.

For a given problem, the researcher needs to choose a method and figure out how far it can go toward modeling the problem of interest.

But, as the previous diagram showed, each method is bound to a scale.

We need to more fully articulate these methods to be able to obtain better results from materials simulations.

Meeting the Challenge of Multiscale: Coupled Methods

- Solutions to the technical challenges are being sought in coupling simulation methods
  - Concurrent coupling / strong coupling needed for tightly coupled problems
    - *Fracture; Electrical Breakdown; Superconductivity; HE Detonation; protein folding & activity; other Biology*
  - Sequential / hierarchical coupling often suffices
    - *Characteristic Lengths & Times do not overlap*
- The essential scientific challenge in coupling simulations is making the transition to the coarser scale
  - Must capture the dominant physical processes -- and not more.

Notes from Previous Slide

At its heart this is **not** an engineering or algorithms issue. It is a science issue:

What averaging can we do to remove the many many unimportant degrees of freedom – the uninteresting details – to be left with just the important degrees of freedom at a coarser scale?

The Sandia multiscale projects are focusing on developing the science of making the links.

Coupled Simulation Methods as BCs

- Couple methods together tightly to use the coaser, less accurate method as boundary constraints (BC) for the higher accuracy method
  - FEM mesh of a continuum as BC for MD
  - Classical MD as BC for Quantum
  - Molecular Continuum as BC for Quantum

Coupled Simulation Methods: Transitions

- Scientific insight is required to devise the needed Transitions between scales and methods:
  - Discrete to thermomechanical Continuum
  - Quantum to Classical
  - Deterministic to Statistical/Stochastic

Notes from Previous Slide

Need to understand the science behind these transitions.

Temperature in discrete systems is average of the vibrations; in continuum it is a field variable.

Developing Coupled Methods to capture Chemistry & Thermomechanics

- Highlight 4 current Sandia projects
  - Modeling Atmospheric Corrosion of Electrical Devices (PI Stephen Foiles, 1834)
  - Developing Multiscale and Reactive Force Field Methods (PI Peter Schultz, 9235)
  - Modeling Local Chemistry in the Presence of Collective Phenomena (PI Normand Modine, 1112)
  - A Coupled Approach for Atomistic-Continuum Simulation (PI Jonathan Zimmerman, 8726)

Notes from Previous Slide

Stephen:

Traditional multiscale from Electronic Structure to continuum, hierarchically.

The three other projects are focusing on developing new transitions.

Peter and Normand's projects are developing systematic approaches to coupling electronic structure to classical atomistics -- one with sequential coupling; the other with concurrent coupling.

Jon's project is aimed at the rest of the scale range from atomistics to thermomechanical continuum.

Simulating Chemistry

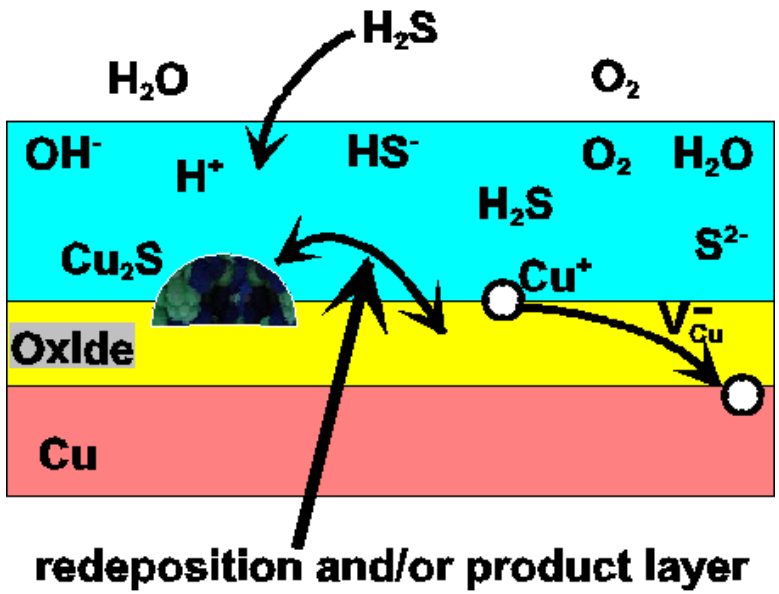
- Current Challenge: Extending force fields to describe reactions (bond breaking and formation)
  - Stephen's approach:
    - *Sequential knowledge transfer. Understanding from atomistic study used to guide modeling in the continuum.*
    - *traditional approach to take for multi-process and rich phenomena.*
  - Peter's approach:
    - *Devise force fields that are reactive*
    - *Fix the parameters using QM calculated "data"*
  - Normand's approach:
    - *Tightly couple QM & MD*
    - *Describe the reaction center quantum mechanically*
    - *Rely on the MD region to capture collective phenom.*

Notes from Previous Slide

Only Stephen is extending chemistry to the continuum.

The other two are aiming to provide systematic approaches that can be applied to a wide range of problems involving reactivity.

Modeling Atmospheric Corrosion of Electrical Devices – S. Foiles



Use Atomistic Simulations and Experiments to generate needed Subgrid-Physics Models

3D multi-phase reaction/diffusion continuum model is needed to simulate real devices and geometry

Multiple Phenomena:

- Adsorption,Speciation, and Reactions, Transport in Liquid Layer
- Gas Phase Transport and Environment
- Liquid Solid Surface Reactions
- Multi-layer solid-state Diffusion

Length Scales:

- Devices (1000 μm)
- Sulfide (1 μm)
- Oxide (0.01 μm)
- Water (0.001 μm)

Time Scales:

- Devices (10^9 sec)
- Atomic (10^-12 sec)

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Notes from Previous Slide

Corrosion (specifically sulfidation of Cu) – the workhorse is continuum model. The challenge is coming up with a good formulation of the continuum model. Look to atomistics for guidance on, e.g., solid state diffusion properties; reaction and action of a few monolayers of water – not a bulk material, hence the thermodynamics differs (effects growth rate dependence on environment);

Continuum phenomena – growth rate of sulfide (reaction rate); morphology, which impacts reactivity and transport in the continuum simulation; gas phase transport; diffusion of Cu through the sulfide and CuO. Need to represent the globally-dependent reaction in a simple form for the continuum.

Stage 1 – thin sulfide layer. Growth dominated by reaction rates at surface.

Stage 2 – thick layer. Growth is limited by diffusion of Cu to the surface.

Pitting of Al is the other most common type of corrosion.

Microscopic understanding used to define the continuum level models

- Surface reaction rates – control of stage I kinetics
  - Form of the constitutive law for surface reactions determined by the microscopic mechanism
  - Need to understand chemistry in *nanoscale* aqueous layers
- Solid State transport – control of stage II kinetics
  - Point defect properties and standard kinetic models
    - *Complex crystal structures makes this very challenging*
    - *Role of impurities?*
- Some unanswered questions for microscopic models
  - Mechanistic origins of corrosion product morphology
  - Explain experimentally observed variation of rates with
    - *Relative humidity*
    - *Light levels*

Significant Challenges at the Continuum Level

- Electrical device-scale simulations performed with ARIA, a 3-D, multiphase, continuum reactive transport code
- Computational challenges for continuum code
  - Multiple phases; Corrosion product morphology
  - Moving boundaries; Globally-dependent reactions
  - Widely disparate length scales and *Long Times*
- Treatment of uncertainty and variability
  - Model/parameter uncertainty and variation in the environment
  - Continuum equations are deterministic for a specific environmental history, initial state, and parameters
    - *Deterministic simulation for a realistic 3D geometry is time-consuming.*
    - *Need to determine probability of failure as a function of time.*

Notes from Previous Slide

Sulfide morphology impacts the reactivity and transport in the continuum simulation.

The corrosion reactions are a BVP in the whole domain, but they need to be represented in the continuum by a simple, local reaction.

Developing Multiscale and Reactive Force Field Methods - P. Schultz

Aim: Integrate atomistic simulation methods to invest fast, versatile semi-empirical methods (MD, TBMD) with quantum accuracy.

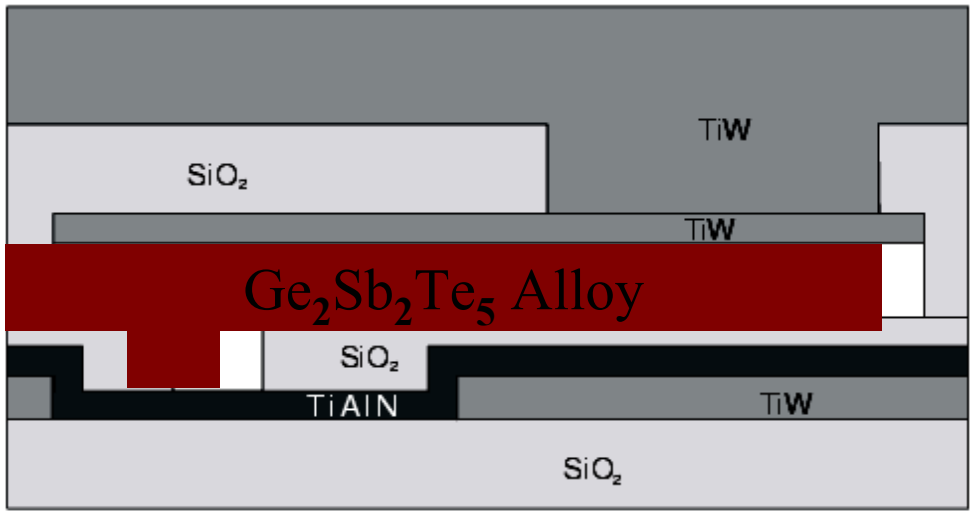
Result: A multiscale materials simulation problem-solving framework and know-how to make use of it.

Test Case: Phase Change Memory Technology

- Non-volatile, Radiation-Hard Memory needed for DOE and Air Force microelectronics applications.
- Electrical analog of optical memory used in CD RW, DVD-RAM and DVD+RW media.
- Small spots of $Ge_2Sb_2Te_5$ alloy rapidly switched between amorphous and crystalline phases.

Non-Volatile C-RAM

- **Simple planar offset structures have been used to investigate basic device physics**



- High endurance
- Long data rentention
- Low voltage, low power
- Compatible with Si chip technology
- Highly scalable
- Enables logic + memory system-on-a-chip

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Target Physics & Chemistry Issues for C-RAM Simulations

- The Phase Transitions
  - Structural: amorphous to poly-crystalline
  - Electronic: semiconducting to metallic
- Switching time (10's of nanoseconds)
- Macroscopic response
  - Delamination?
  - Material compatibilities?

Notes from Previous Slide

Plan is to apply a semi-empirical method like MD for large scale simulations that can be used to investigate these questions, once the atomistic method has been endowed with reactivity and quantum accuracy.

The Material Modeling Process

Development and parameterization of RFF MD & TBMD:

1) Choose the physics needed in the simulation.
2) Identify atoms and other particles.
3) Choose parameterization of the physics.
4) Generate Training Sets of material property values ("data")
5) Perform internal validation.
6) Apply calibrated semi-empirical method.
7) Augment with full quantum calculations, where needed.

Notes from Previous Slide

1) What phys/chem do you want the SE simulation to predict?

   Bond breaking/making; band gaps; phase transformations; temperature dependent properties?

   Can't use standard MD for bond breaking/making

2) Which atoms are important? Unified atom repr? Need explicit impurities?

   Factorial fitting or worse.

3) Meaning of parameters? Non-SC or SC TB w/ charge xfer. Latter is new and requires lots of code and TB method development, but would provide higher fidelity.

   FFs parameterization is wide open – multiply different 1, 2, & 3 body interactions, charge xfer. Expect to have lots of parameters and new forms for RFFs unlike any existing currently in LAMMPS.

4) Need a set of data that spans all of the space of properties & fundamental phenomena (the physics) that you hope to include in the S-E simulations.

   Include all possible structural data (energies, bond lengths, lattice constants – all for many structures), elastic properties, far from equilibrium energies, band gaps. Also need info on properties of any reactants and products of interest.

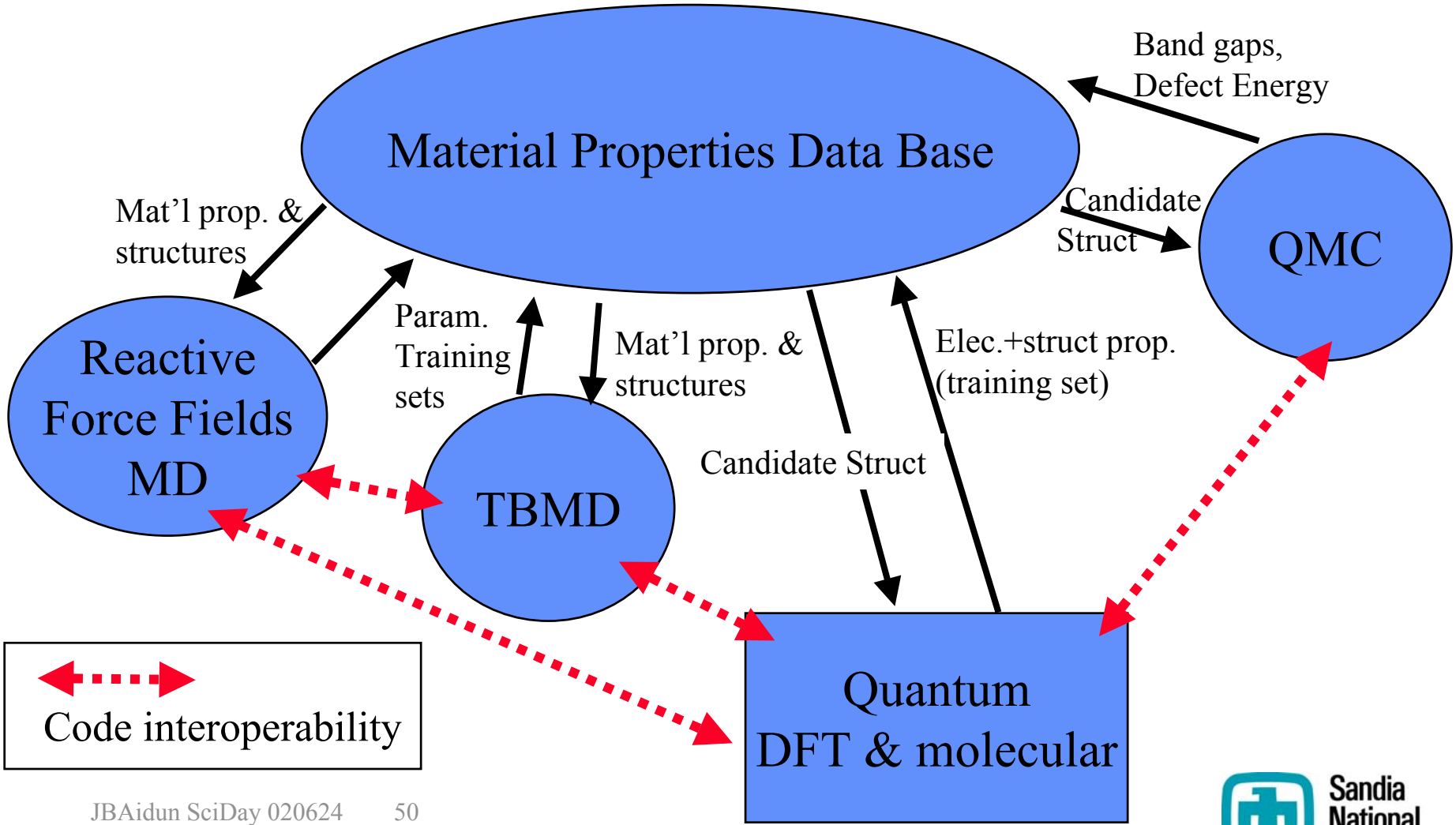
[the process amounts to a giant interpolation functional, in some sense]

5) Reserve some distinct test cases for validation

6) Crystal thermal properties, interfaces, defects, amorphous systems + w/ defects & interfaces, phase transformations, reactions (HE).

7) Where the physics in the data set is suspect or insufficient, do QM.

Material Modeling Tool Set



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Notes from Previous Slide

The point here is that there is a substantial flow of information between the methods and it will be highly automated thru loose coupling of the codes – “interoperability.”

Challenges to Simulating C-RAM

- Complex physics
  - Phase transitions: Structural & Electronic
    - *Likely to be coupled → electronic/thermally driven*
  - Electronic properties are critical for accuracy
  - Extended time scale (10's of ns): pushes ability of classical MD; beyond the range of TBMD
- Simulation Methods
  - New formulations for force fields to portray the Chemistry
  - New multi-component/multi-phase TBMD
  - Codes need to be interoperable (loosely coupled)
  - Big simulations needed in QM, TBMD, and MD

Notes from Previous Slide

Electronic properties, like band gaps, are hard to calculate accurately.
We hope to be able to use QMC for such calculations.

Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

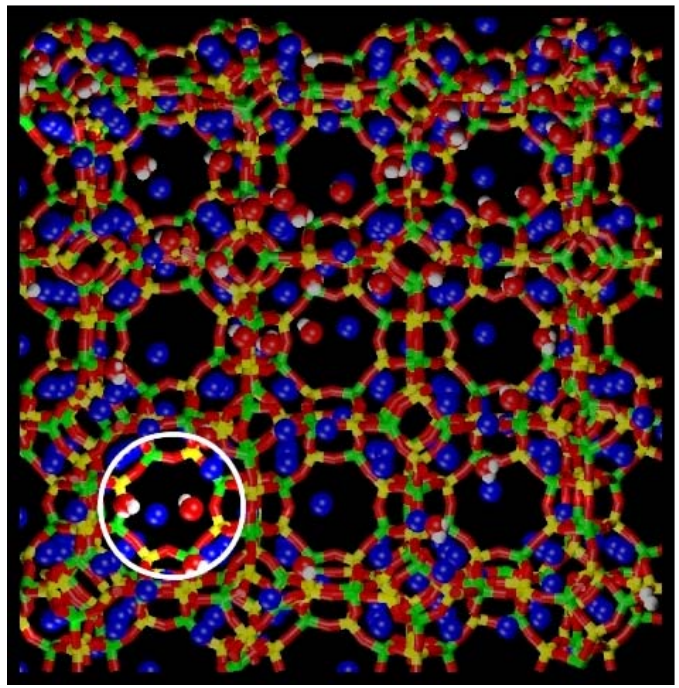
Aim: Model local Chemistry in the presence of Collective Phenomena to advance scientific understanding of complex materials

Test case: Absorbtion in Zeolite desiccant

Approach: Couple Green's Function Electronic Structure method to classical MD

- Exploits localized nature of ES.
- Transition: "anchored" orbital BC on QM region facilitate embedding in classical MD region.
- Update ion positions in QM region after every MD time step.

Result: A flexible, production-level multiscale modeling tool for materials science.



Zeolite: nano-porous alumino-silicate + Na^+

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Notes from Previous Slide

Zeolite desiccant is used in the stockpile to suppress oxidation and hydration.

Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

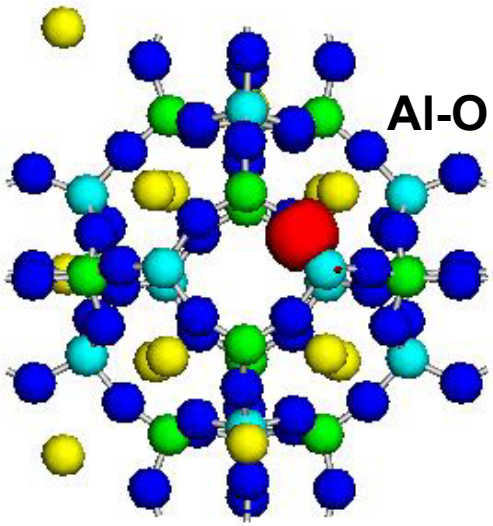
- Issues:
  - Adapting the QDFT method to keep the Green's function matrix manageably small.
  - Energy conservation.
  - QM region needs to be just a few atoms (say, 5) to be able to sample the long times on which collective phenomena occur
    - *Highly dependent on having a good transition.*
  - Update of anchored orbitals in transition region
    - *How often is it needed?*
    - *How accurate does it need to be?*

Notes from Previous Slide

The significance of a lack of energy conservation varies with the application from being a nuisance to being a show stopper.

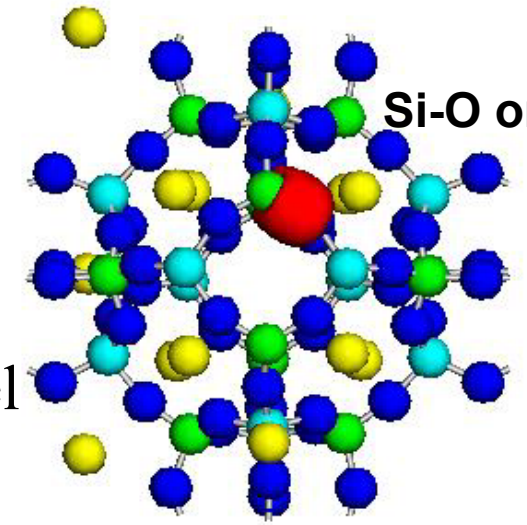
Modeling Local Chemistry

- First Year's Progress: Efficient GFES method implemented.
- Multiscale method enables study of electron distribution in the structure.



Al-O orbital

Zeolite model structure



Si-O orbital

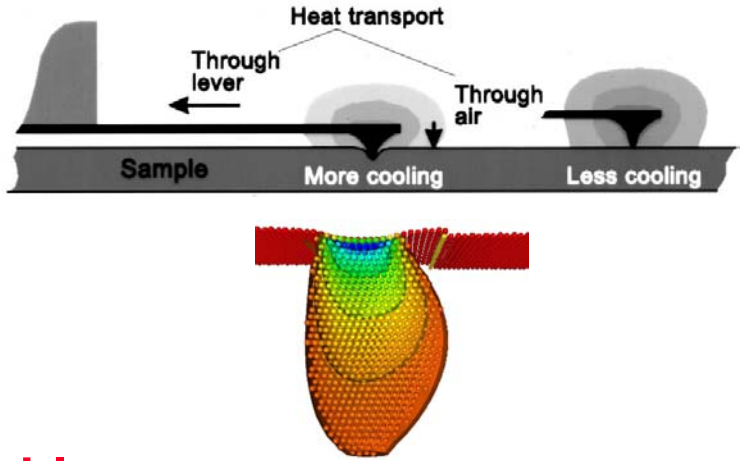
[O: dk blue, Al: lt blue, Si: green, H: red, Na: yellow]

Modeling Local Chemistry in the Presence of Collective Phenomena – N. Modine

- Advantages:
  - Natural, nearly seamless coupling of QM to MD.
    - *No need to artificially terminate bonds.*
    - *Good balance of comput'l effort between QM & MD.*
  - Thermal energy transfers between regions.
  - Collective Phenom. of MD region influence chemistry in QM region thru transmitted strains and E-Field
  - Good parallel scaling.
  - Amenable to adaptively spawning QM regions.
  - Prototype for class of confined reaction problems
    - *Catalysis*
    - *in vivo reactions (enzyme moderated)*
    - *Reactivity in nanotechnological settings*

A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman

(Binning et al.; 1999)



Problem:

Sandia designs and manufactures devices that exhibit multiple modes of material failure, e.g. brittle fracture and plasticity, at various length scales. Models are needed to provide accurate predictions of material reliability.

Aim:

Develop a simulation methodology that contains *atomistics* to model the defect-related mechanisms operating at the nano-scale and *continuum mechanics* to simulate micro- and macro-scale geometries.

Result:

Modeling capability that efficiently and consistently conveys fine-scale detail up to a macroscopic continuum simulation of material response.

Test Case:

AFM data storage by thermo-mechanical indentation

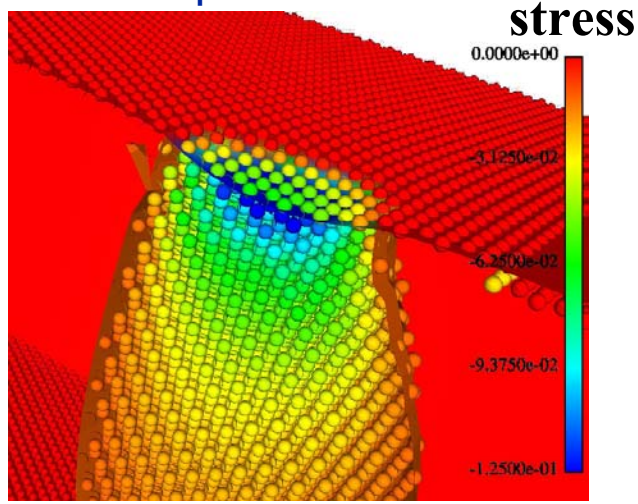
Notes from Previous Slide

Sandia has numerous projects focusing on the material modeling of microsystem components. Various efforts exist, e.g. LIGA, SMM and MEMS, that are centered on the design and manufacture of microdevices. These devices show multiple modes of material failure at various length scales that need to be modeled for accurate reliability predictions. Possible failure modes consist of brittle fracture, ductile fracture, plasticity/dislocation activity, grain boundary sliding, stiction, friction and wear.

A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman

Technical Approach:

- Develop compatible definitions for stress, deformation and temperature for both domains.
- Formulate proper interface conditions between the domains.
- Perform an analysis on wavelength-dependent energy content for mechanical deformation of atomistic systems.
- Partition the energy transferred between a dynamic atomistic system and a finite element mesh into elastic waves and a temperature field.



Applications:

- Simulations of experiments used to obtain material properties - e.g. nanoindentation.
- Fundamental understanding of the thermo-mechanical behavior of material defects.
- Mechanical analysis of nano-scale deformation during friction, stiction and wear.

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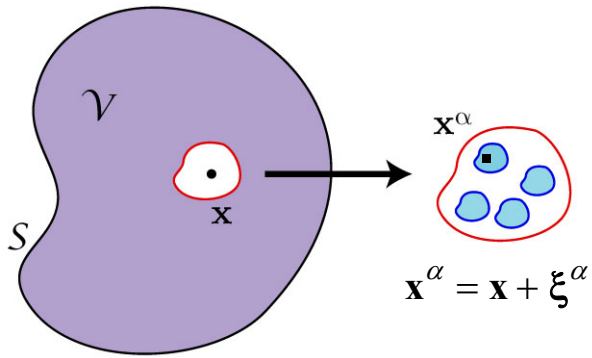
Notes from Previous Slide

Partitioning the energy between elastic waves and temperature in the continuum is a very big challenge.

A Coupled Approach for Atomistic-Continuum Simulation – J. Zimmerman

First Year's Progress:

- Evaluated atomistic definitions of stress for consistency with continuum
- Extended micropolar continuum theory to provide transition between atomistics and continuum:
  - *A structured continuum with additional internal degress of freedom.*



- Developed a hybrid gridding method to manage load balancing for coupled atomistic-continuum simulations on MP computers.

Notes from Previous Slide

The additional DOFs of the micropolar continuum should facilitate the transition from atomistics to traditional continuum.

The Further Challenge: Activated Processes

- Identifying Transition States is the key for capturing Diffusion, Reactivity, and Chemistry in simulations.
- Transition State finding is computionally intensive.
- Transition States determine Chemical Specificity but are dependent on system dynamics (Collective Phenomena)
  - How to couple these in a simulation?
- Transitions are infrequent and sparse
  - Their time and location are not known.
  - Quantum accuracy will be required, usually
- The Next Goal: Adaptively apply QM & find Transition States when and where they are needed within a large, classical MD system.

Notes from Previous Slide

Coupling transition states to dynamics is a near-term issue for Normand's project.

Sometimes we know what the system is going to do.

More often we don't, or worse, we think we know what it will do but are wrong.

A Current Challenge for Quantum DFT – Improving Treatment of Many-Body Effects

- QDFT is the workhorse method providing the underpinnings of multiscale materials simulation
- QDFT is exact, . . . in theory.
- Sandia National Laboratories Workshop To spur progress in developing better EXC functionals:

Quantum Mechanical Techniques: Exchange - Correlation Functionals in Density Functional Theory

- 14-16 August 2002 at the Wyndham Hotel, Albuq.
- Sponsored by the Computer Science Research Institute and the Physical & Chemical Sciences Center
- Ann Mattsson, Organizer

Notes from Previous Slide

A final note –

Quantum calc'ns are hard but they provide the crucial underpinnings of multiscale materials simulations.

The workhorse method, DFT is highly accurate for a range of applications, but its treatment of the many-body effects of the collection of electrons is too approximate for problems that increasingly concern us: surfaces and interfaces, vacancy defects, and transition states – all important for simulating chemistry and reactivity.

To spur progress in developin better treatments of many-body effects, Ann Mattsson is organizing a workshop for the world experts in this field.

We are looking forward to a stimulating exchange of ideas and brainstorming with potential world-wide impact.

THANKS!
to many colleagues for contributions

- Physical & Chemical Sciences, 1100
  - Normand Modine
  - Ann Mattsson
  - Alan Wright, Kevin Leung
  - J. Charles Barbour
  - Neal Shinn
- Materials & Process Sciences, 1800
  - Stephen Foiles
  - Michael Chandross
  - H. Eliot Fang
  - Jeffrey Hoyt
- Engineering Sciences, 9100
  - Bob Chambers
  - James Cox
  - E. David Reedy
  - Arne Gullerud
  - Terry Hinnerichs
- Materials & Engineering Sci.s, 8700
  - Jon Zimmerman
  - Mark Horstemeyer
- Geoscience & Environment, 6100
  - Louise Criscenti
  - Henry Westrich
- Pulsed Power Sciences, 1600
  - Michael Desjarlais
- Computation, Computers, Information & Mathematics, 9200
  - Peter Schultz
  - Steven Plimpton
  - Mark Sears